

Spin-splitting surface states of strained GaAs(001) and spontaneous spin current from breaking of twofold symmetry



Tomonori Iijima*

3028-1-312 Nogawa, Miyamae-ku, Kawasaki, Kanagawa 216-0001, Japan

ARTICLE INFO

Article history:

Received 2 June 2015

Accepted 18 August 2015

Available online 29 August 2015

Keywords:

Spin splitting

Spin current

Strain-induced spin-orbit coupling

ABSTRACT

We theoretically study the electronic structure and spin splitting of a strained GaAs(001) surface with broken twofold symmetry. We introduce a surface electron Hamiltonian of our model. By $\mathbf{k} \cdot \mathbf{p}$ theory, we qualitatively evaluate the electronic structure of GaAs(001) surface, demonstrating that the spin degeneracy of the bottom of the surface-state conduction bands is split. Additionally, by the spin current operator, we evaluate the spin current of electrons in the bottom of the surface-state conduction bands, demonstrating that for n-type GaAs the spin current flows in the parallel direction to a mirror plane spontaneously. This is a new mechanism to generate the spin current.

© 2015 The Author. Published by Elsevier B.V. This is an open access article under the CC BY-NC-ND license (<http://creativecommons.org/licenses/by-nc-nd/4.0/>).

1. Introduction

Ever since the intrinsic spin Hall effect was proposed [1,2], interest in spin properties has increased. The intrinsic spin Hall effect, proposed by Sinova et al. [1], originates from Rashba-type spin splitting. Materials that exhibit giant Rashba-type spin splitting is desirable for fabricating many semiconductor-based spintronic devices currently being studied [3]. Spin splitting occurs when inversion symmetry is broken, a behavior that can arise in five cases: first, when a crystal lacks a center of inversion in the bulk [4], in two-dimensional electronic states with structural inversion asymmetry [5], at surfaces that lack three-dimensional symmetry [6], at interfaces of semiconductor heterostructures at which chemical bonding is asymmetric [7,8], and at surface alloys on metals and an adlayer on semiconductor substrates with in-plane inversion asymmetry [9–12]. Though up to now in-plane inversion asymmetry is due to missing of one mirror plane by alloying or adsorbing, we introduce in-plane inversion asymmetry by applying stress at the topmost surface. We wish to search for novel spin properties at surfaces with in-plane inversion asymmetry.

In this paper we theoretically consider spin-splitting surface states from breaking of the inversion symmetry of the surface in GaAs, a zinc blende crystal. Our model is based on that of the quantum spin Hall effect, proposed by Bernevig and Zhang [13]. In their model, the quantum spin Hall effect is induced by the shear strain

gradients in a quantum well that has the mesoscopic twofold symmetry of the interface. In contrast, in our model the mesoscopic twofold symmetry of the topmost surface of GaAs(001) is broken. Additionally, we discuss a novel phenomenon which can be utilized as a new mechanism to generate the spin current.

2. Theory

Assessing the conduction bands of strained zinc blende crystals, in the framework of perturbation theory, an electron Hamiltonian can be written as [14–18]

$$\begin{aligned} H &= H_0 + H_S + H_{SO}, \\ H_0 &= \frac{1}{2m} \mathbf{p}^2 + V_0(\mathbf{x}), \\ H_S &= a(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}), \\ H_{SO} &= \frac{\hbar}{2} \{ (\sigma \Omega_D) + (\sigma \Omega_{S1}) + (\sigma \Omega_{S2}) \}, \end{aligned} \quad (1)$$

where m is the bare electron mass, $V_0(\mathbf{x})$ is the potential in the unstrained crystals, a is the hydrostatic deformation potential, ε_{ij} is the strain tensor component, and σ are Pauli matrices. Additionally, in the perturbative Hamiltonian H_{SO} , the first term describes the Dresselhaus spin-orbit coupling, while the second and third terms describe the strain-induced spin-orbit coupling. The Dresselhaus spin-orbit coupling originates from the periodic potential in the crystal, while the strain-induced spin-orbit coupling originates from the potential in the strained crystal. Ω_D , Ω_{S1} and Ω_{S2} are vectors with components

* Tel.: +81 44 797 2573.

E-mail address: ijima@or2.fiberbit.net

$$\begin{aligned}\hbar\Omega_{Dx} &= \alpha E_g^{-1/2} p_x(p_y^2 - p_z^2), \\ \hbar\Omega_{S1x} &= v(\varepsilon_{xy}p_y - \varepsilon_{xz}p_z), \\ \hbar\Omega_{S2x} &= v'p_x(\varepsilon_{yy} - \varepsilon_{zz}).\end{aligned}\quad (2)$$

The remaining components of these vectors are obtained by cyclic permutation of the indices x , y , and z . In Eq. (2) E_g is the width of the band gap, and α , v and v' are constants that determine the magnitude of the spin-orbit coupling. It is reasonable that H_{SO} can be written as Eqs. (1) and (2), because H_{SO} is invariant, consisting of basis sets for the irreducible representation Γ_5 of group T_d [16]. Experiments by Wu et al., investigating strain-induced spin-orbit coupling, indicated that for GaAs the strain-induced spin-orbit coupling is more important than the Dresselhaus spin-orbit coupling [19]. The constants v and v' of the strain-induced spin-orbit coupling are 8×10^5 (m/s) and 6×10^5 (m/s) for bulk GaAs [13,19], respectively.

We describe our model below. We choose one of the topmost lattice points of an ideal surface as the origin of the coordinate system and x , y , and z axes along the $[100]$, $[010]$, and $[001]$ direction, respectively. Modifying Bernevig and Zhang's model [13], we apply strain at the topmost surface by shifting the topmost surface atoms from its ideal surface position, described as

$$\mathbf{u} = (u_x, u_y, u_z) = (0, 0, T(y)2gxy), \quad (3)$$

where g is a constant that determines the magnitude of the displacement, and $T(y)$ is an operator and defined as

$$T(y)f(y) = \begin{cases} f(-y) & \text{if } y \geq 0 \\ f(y) & \text{otherwise,} \end{cases}$$

where $f(y)$ is an arbitrary function. Our above model differs from that of Bernevig and Zhang by operating $T(y)$ on u_z [13]. Modifying further, we use the strain tensor components of the small inhomogeneous confined strain, as described by

$$\begin{aligned}\varepsilon_{xx} &= \varepsilon_{yy} = \varepsilon_{zz} = 0, \\ \varepsilon_{xy} &= \varepsilon_{yx} = 0, \\ \varepsilon_{yz} &= \varepsilon_{zy} = S(y)gx \exp[-\alpha\sqrt{x^2 + y^2}] \exp[-n^2z^2], \\ \varepsilon_{zx} &= \varepsilon_{xz} = T(y)gy \exp[-\alpha\sqrt{x^2 + y^2}] \exp[-n^2z^2], \\ S(y)f(y) &= \left(\frac{\partial T(y)}{\partial y}\right)f(y) = \begin{cases} -f(y) & \text{if } y \geq 0 \\ f(y) & \text{otherwise,} \end{cases}\end{aligned}\quad (4)$$

where α is a positive appropriate constant and n is a large enough integer. Here, GaAs is in the region $z \geq 0$, while the region $z < 0$ corresponds to the vacuum. Fig. 1 shows the displacement of the

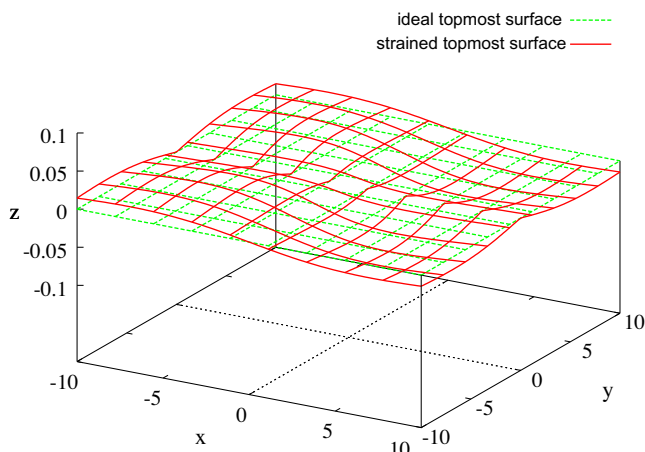


Fig. 1. Displacement of the topmost surface atoms of the topmost surface of strained GaAs(001). The origin is one of the topmost lattice points of the ideal surface. x , y , and z axes are along the $[100]$, $[010]$, and $[001]$ direction, respectively.

topmost surface atoms. Thus, in our model the mesoscopic twofold symmetry of the strained GaAs(001) surface is broken. We treat the effect of the displacement of the topmost surface atoms as a perturbation of the potential [20]. Here, the strain given by Eq. (4) can be realized by applying tensile stress within the first and fourth quadrants of the xy -plane at the topmost surface as well as compressive stress within the second and third quadrants of the xy -plane at the topmost surface, with fixed atoms on the x and y axes. By reconstruction of GaAs(001) surface, the distortion appears because of dimerization or dimer buckling. However, no strain is generated by representative reconstructions of the GaAs(001) surface, including the $c(4 \times 4)$ reconstruction and the 2×4 reconstruction. Thus, the strain tensor components (4) describe the strain of the strained GaAs(001) surface of our model if we consider reconstructions. Here, in the perturbative Hamiltonian H' in Eq. (1), the first term, which describes the Dresselhaus spin-orbit coupling, can be omitted because the surface has a center of inversion in xy -plane. Additionally, H_S and the third term in H_{SO} does not contribute to H , because $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = 0$. Therefore, the surface electron Hamiltonian of our model can be written as

$$\begin{aligned}H &= H_0 + H_{SO}, \\ H_0 &= \frac{1}{2m}\mathbf{p}^2 + V_0(\mathbf{x}), \\ H_{SO} &= \frac{\hbar}{2}(\sigma_x\Omega_{S1x} + \sigma_y\Omega_{S1y} + \sigma_z\Omega_{S1z}),\end{aligned}$$

where

$$\begin{aligned}\hbar\Omega_{S1x} &= -vgT(y) \exp[-\alpha\sqrt{x^2 + y^2}] \exp[-n^2z^2]yp_zT^{-1}(y), \\ \hbar\Omega_{S1y} &= vgS(y) \exp[-\alpha\sqrt{x^2 + y^2}] \exp[-n^2z^2]xp_zS^{-1}(y), \\ \hbar\Omega_{S1z} &= vgT(y) \exp[-\alpha\sqrt{x^2 + y^2}] \exp[-n^2z^2](yp_x - xp_y)T^{-1}(y),\end{aligned}$$

and $V_0(\mathbf{x})$ is the potential in the ideal unstrained surface. The region $z \geq 0$ corresponds to the semi-infinite lattice. This perturbative Hamiltonian H_{SO} only has a substantial effect near the topmost surface in z direction on the surface electron Hamiltonian. Because $\langle \alpha|\sigma_i|\alpha \rangle = \langle \beta|\sigma_i|\beta \rangle = 0$ ($i = x, y$), we can simply consider the perturbative Hamiltonian H'_{SO} now.

$$\begin{aligned}H'_{SO} &= \frac{\hbar}{2}\sigma_z\Omega_{S1z} \\ &= \frac{1}{2}vg \exp[-\alpha\sqrt{x^2 + y^2}] \exp[-n^2z^2]T(y)(yp_x - xp_y)T^{-1}(y)\sigma_z.\end{aligned}$$

Here, $\hbar\Omega_{S1x}$ and $\hbar\Omega_{S1y}$ are hermitian because

$$\begin{aligned}\frac{d \exp[-n^2z^2]}{dz} &= -2n^2z \exp[-n^2z^2] \\ &= 2\left\{\delta(z + (1/\sqrt{2}n)) - \delta(z - (1/\sqrt{2}n))\right\}.\end{aligned}$$

and because the wave function is continuous at $z = 0$ in z direction. We use this Hamiltonian $H = H_0 + H'_{SO}$ to evaluate the electronic structure.

3. Results and discussion

We now qualitatively evaluate the electronic structure of surface-state conduction bands near the Γ point. Assuming a small perturbation, we consider that the surface electron is in Bloch states in the x and y directions as $\Psi_{\mathbf{k}_\parallel}(\mathbf{x}) = \exp[i\mathbf{k}_\parallel \cdot \mathbf{x}]u_{\mathbf{k}_\parallel}(\mathbf{x})$ ($\mathbf{k}_\parallel = (k_x, k_y)$) in the region $z \geq 0$. The function $u_{\mathbf{k}_\parallel}(\mathbf{x})$ satisfies the equation,

$$\left[\frac{1}{2m}\mathbf{p}^2 + V_0(\mathbf{x}) + \frac{\hbar^2\mathbf{k}_\parallel^2}{2m} + \frac{\hbar}{m}k_xp'_x + \frac{\hbar}{m}k_y p'_y + H'_{SO}\right]u_{\mathbf{k}_\parallel}(\mathbf{x}) = E(\mathbf{k}_\parallel)u_{\mathbf{k}_\parallel}(\mathbf{x}),$$

where

$$p'_x = p_x + \frac{m}{\hbar} \frac{1}{2} v g h \exp[-\alpha \sqrt{x^2 + y^2}] \exp[-n^2 z^2] T(y) y T^{-1}(y) \sigma_z,$$

$$p'_y = p_y - \frac{m}{\hbar} \frac{1}{2} v g h S(y) \exp[-\alpha \sqrt{x^2 + y^2}] \exp[-n^2 z^2] x S^{-1}(y) \sigma_z.$$

Here, in the region $z \geq 0$ $u_s(\mathbf{x}) = f_s(r)$, $u_x(\mathbf{x}) = x f_p(r)$, and $u_y(\mathbf{x}) = y f_p(r)$ satisfy the equation

$$\left[\frac{1}{2m} \mathbf{p}^2 + V_0(\mathbf{x}) \right] u_s(\mathbf{x}) = E_s(\mathbf{0}) u_s(\mathbf{x}),$$

$$\left[\frac{1}{2m} \mathbf{p}^2 + V_0(\mathbf{x}) \right] u_i(\mathbf{x}) = E_p(\mathbf{0}) u_i(\mathbf{x}) \quad (i = x, y),$$

under the condition that in the region $z < 0$ $V_0(\mathbf{x}) = V'_0$ (V'_0 is infinitely high.), where $E_s(\mathbf{0})$ and $E_p(\mathbf{0})$ are the energy eigenvalue of the s band of the surface-state conduction bands at the Γ point and that of the p band of the surface-state valence bands at the Γ point, respectively. We expand the wave function of the s band of surface-state conduction bands at $\mathbf{k}_{\parallel} = \tilde{\mathbf{k}}_{\parallel}$ near the Γ point $u_s^{(s)}(\mathbf{x})$

by $u_i(\mathbf{x}) (i = s, x, y)$ by using $\mathbf{k} \cdot \mathbf{p}$ theory [21]. Then, we evaluate the energy eigenvalue of the s band of the surface-state conduction bands at $\mathbf{k}_{\parallel} = \tilde{\mathbf{k}}_{\parallel}$ near the Γ point $E_s(\tilde{\mathbf{k}}_{\parallel})$ by $\mathbf{k} \cdot \mathbf{p}$ theory. We do not consider dangling bonds of the topmost surface atoms, and we assume that bonding between adjacent (001) plane is weak. Additionally, we do not consider reconstruction of GaAs(001) surface. Up to the third order in energy, we obtain

$$E_s(\tilde{\mathbf{k}}_{\parallel}) = E_s(\mathbf{0}) \mp C_{k_x}^{(1)} \tilde{k}_x + C_{k_x}^{(2)} \tilde{k}_x^2 + C_{k_y}^{(2)} \tilde{k}_y^2 \mp C_{k_x}^{(3)} \tilde{k}_x^3 \pm C_{k_x}^{(4)} \tilde{k}_x \tilde{k}_y^2, \quad (5)$$

where

$$C_{k_x}^{(1)} = \frac{2\sqrt{\pi} v g h}{n} \int_0^\infty \{f_s(r)\}^2 \exp[-\alpha r] r^2 dr,$$

$$C_{k_x}^{(2)} = C_{k_y}^{(2)} = \left\{ \frac{\hbar^2}{2m} + \left(\frac{\hbar}{m} \right)^2 \frac{|\langle x | p_x | s \rangle|^2}{E_s(\mathbf{0}) - E_p(\mathbf{0})} \right\},$$

$$C_{k_x}^{(3)} = \frac{2\sqrt{\pi} v g h}{n} \left(\frac{\hbar}{m} \right)^2 \frac{|\langle x | p_x | s \rangle|^2}{\{E_s(\mathbf{0}) - E_p(\mathbf{0})\}^2} \cdot \left[\frac{1}{3} \int_0^\infty \{f_p(r)\}^2 \exp[-\alpha r] r^4 dr - \int_0^\infty \{f_s(r)\}^2 \exp[-\alpha r] r^2 dr \right],$$

$$C_{k_x}^{(4)} = \frac{2\sqrt{\pi} v g h}{n} \left(\frac{\hbar}{m} \right)^2 \frac{|\langle x | p_x | s \rangle|^2}{\{E_s(\mathbf{0}) - E_p(\mathbf{0})\}^2} \cdot \int_0^\infty \{f_s(r)\}^2 \exp[-\alpha r] r^2 dr,$$

$$\langle x | p_x | s \rangle = \int u_x^*(\mathbf{x}) \frac{\hbar}{i} \frac{\partial}{\partial x} u_s(\mathbf{x}) d\mathbf{x},$$

and the upper sign and lower sign denote the upspin and downspin, respectively. Here, we use $\exp[-n^2 z^2] = \exp[-n^2 (r \cos \theta)^2] = (\sqrt{\pi}/n) \delta_n(r \cos \theta)$ ($\delta_n(t)$ is a delta sequence.). Thus, the spin degeneracy of the bottom of the surface-state conduction bands is split. Figs. 2 and 3 show schematics of the electronic structure of the bottom of the surface-state conduction bands. Here, the spin-splitting is caused by the dependence of the spin direction in the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian. However dangling bonds rebound, and however GaAs(001) surface is reconstructed, the wave function spreads in the (001) planes. Thus, the obtained electronic structure gives a qualitative insight into the real electronic structure of strained GaAs(001) surface with broken twofold symmetry.

Now, we discuss a model similar to Bernevig and Zhang's model [13]. In this model, the perturbative Hamiltonian $H_{SO}^{(B-Z)}$ is given as

$$H_{SO}^{(B-Z)} = (1/2) v g \exp[-\alpha \sqrt{x^2 + y^2}] \exp[-n^2 z^2] (y p_x - x p_y) \sigma_z.$$

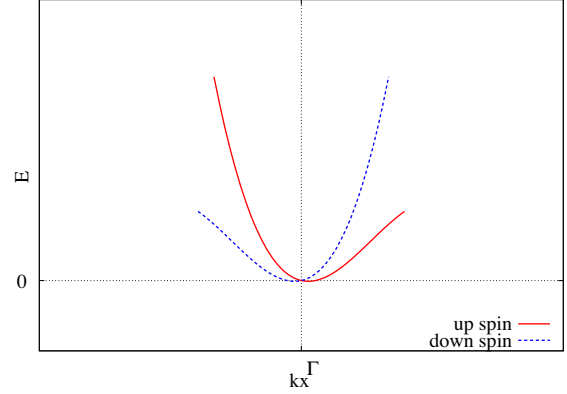


Fig. 2. Schematic of the electronic structure of the bottom of strained GaAs(001) surface-state conduction bands in our model. This figure is plotted along the k_x axis. $C_{k_x}^{(3)}$ is assumed to be positive.

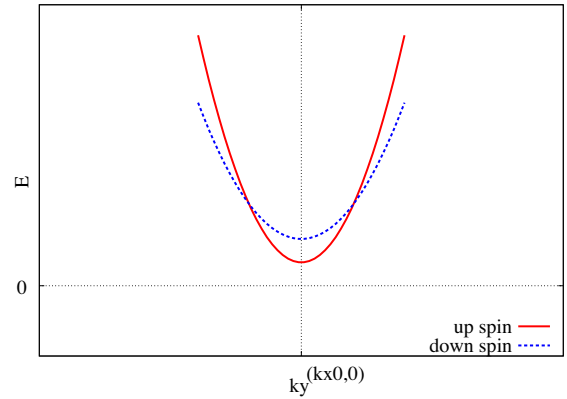


Fig. 3. Schematic of the electronic structure of the bottom of strained GaAs(001) surface-state conduction bands in our model. This figure is plotted along $\mathbf{k}_{\parallel} = (k_{x0}, k_y)$ (k_{x0} is a positive constant.). $C_{k_x}^{(3)}$ is assumed to be positive.

We evaluate the energy eigenvalue of the s band of the surface-state conduction bands of the model similar to Bernevig and Zhang's model near the Γ point $E_s^{(B-Z)}(\tilde{\mathbf{k}}_{\parallel})$ by $\mathbf{k} \cdot \mathbf{p}$ theory. Up to the third order in energy, we obtain $E_s^{(B-Z)}(\tilde{\mathbf{k}}_{\parallel})_{\uparrow} = E_s(\mathbf{0}) + a(\tilde{k}_x^2 + \tilde{k}_y^2)$ (a is a positive constant.); that is,

$$E_s^{(B-Z)}(-\tilde{\mathbf{k}}_{\parallel})_{\uparrow} = E_s^{(B-Z)}(\tilde{\mathbf{k}}_{\parallel})_{\uparrow}. \quad (6)$$

Thus, the spin degeneracy of the surface-state conduction bands of the model similar to Bernevig and Zhang's model is not split.

Here, we compare in-plane inversion asymmetry of surface alloys on metals and an adlayer on semiconductor substrates with that of our model. As for the former, by a nearly-free electron (NFE) model [9] and $\mathbf{k} \cdot \mathbf{p}$ theory in addition to symmetry analyses [12] it is demonstrated that in-plane inversion asymmetry makes the Rashba type dispersion relations anisotropic and induces the spin polarization in the normal direction to the surface. Besides, the interplay of structural inversion asymmetry (in the normal direction to the surface) and in-plane inversion asymmetry enhances splitting [9]. As for the latter, we use strain-induced spin-orbit coupling derived by in-plane inversion asymmetry (broken twofold symmetry) and $\mathbf{k} \cdot \mathbf{p}$ theory and demonstrate that strain-induced spin-orbit coupling makes the dispersion relations anisotropic and induces spin splitting of eigenstates of spin operator σ_z .

In addition, we mention the difference between spin splitting induced by heterostructural interface asymmetry and that by our model. The former is caused by the following reason. At interfaces

of zinc blende based semiconductor heterostructures grown along the [001] axis, atomic structures, whose threefold symmetry is broken, have D_{2d} symmetry because of “common anion”. On the other hand, in “no common atom” heterostructures such as C1A1/C2A2 (C1 and C2 are cations, and A1 and A2 are anions.), there are two inequivalent interfaces to correspond to C1–A1–C2 and C2–A2–C1. Thus, atomic structures at interfaces have lower C_{2v} symmetry, so that tight-binding calculations, which consider the full symmetry, explained optical anisotropy [22]. Additionally, in the framework of the envelope function approximation the “ H_{BF} model” and the generalized boundary conditions demonstrated spin splitting of heavy hole or light hole subbands [7] and that of electron subbands [23], respectively. Here, in “ H_{BF} model” two operators B and F corresponding to ‘backward’ and ‘forward’ bonds on each side of a C–A–C’ monolayer (C and C’ are cations and A is an anion.) are introduced and an asymmetric potential is added to the Hamiltonian as the perturbation [24]. In the generalized boundary conditions originally the term describing the heavy-light hole mixing due to the C_{2v} symmetry is added to the Hamiltonian and the boundary conditions are changed [25]. On the other hand, we assume that the surface is not reconstructed and that atomic structures have T_d symmetry, and we qualitatively evaluate the electronic structure by $\mathbf{k} \cdot \mathbf{p}$ theory.

Now, we discuss electron-doped n-type GaAs. In this case, the surface-state conduction bands are filled by electrons from lower to higher energy levels. Here, the expectation value of the velocity of an electron in a Bloch state of the n band is given as $\mathbf{v}^{(n)}(\mathbf{k}) = 1/\hbar \partial E_n(\mathbf{k}) / \partial \mathbf{k}$ ($E_n(\mathbf{k})$ is the energy eigenvalue of the n band.), using Feynman’s theorem. Because $\mathbf{v}^{(n)}(\mathbf{k}) = 1/\hbar \partial E_n(\mathbf{k}) / \partial \mathbf{k}$ in addition to Figs. 2 and 3, the spin current in x direction is to be expected. In our model, using the spin current operator $j_i^z = (1/2)\{v_i, s_x\}$ (v_i and s_x are the velocity and spin operator, respectively.), we evaluate the spin current in the x direction of the s band electron $j_x^{(s)}$ and that in the y direction of the s band electron $j_y^{(s)}$ over Bloch states with the energy eigenvalue less than E_F near Γ point. Assuming that the Fermi surface is a circle with the radius of k_F , we obtain

$$\begin{aligned} j_x^{(s)} &= \sum_{\mathbf{k}_\parallel} \left\{ \frac{\hbar}{2} v_x^{(s)}(\tilde{\mathbf{k}}_\parallel)_\uparrow \theta(E_F - E_s(\tilde{\mathbf{k}}_\parallel)_\uparrow) - \frac{\hbar}{2} v_x^{(s)}(\tilde{\mathbf{k}}_\parallel)_\downarrow \theta(E_F - E_s(\tilde{\mathbf{k}}_\parallel)_\downarrow) \right\} \\ &= \left(\frac{L}{2\pi} \right)^2 \int \frac{\hbar}{2} \left\{ \frac{1}{\hbar} \frac{\partial E_s(\tilde{\mathbf{k}}_\parallel)_\uparrow}{\partial k_x} \theta(E_F - E_s(\tilde{\mathbf{k}}_\parallel)_\uparrow) \right. \\ &\quad \left. - \frac{1}{\hbar} \frac{\partial E_s(\tilde{\mathbf{k}}_\parallel)_\downarrow}{\partial k_x} \theta(E_F - E_s(\tilde{\mathbf{k}}_\parallel)_\downarrow) \right\} d\tilde{k}_x d\tilde{k}_y \\ &= \frac{L^2}{4\pi} \left(-C_{k_x}^{(1)} k_F^2 - \frac{3}{4} C_{k_x}^{(3)} k_F^4 + \frac{1}{4} C_{k_x}^{(4)} k_F^4 \right), \\ j_y^{(s)} &= \sum_{\mathbf{k}_\parallel} \left\{ \frac{\hbar}{2} v_y^{(s)}(\tilde{\mathbf{k}}_\parallel)_\uparrow \theta(E_F - E_s(\tilde{\mathbf{k}}_\parallel)_\uparrow) - \frac{\hbar}{2} v_y^{(s)}(\tilde{\mathbf{k}}_\parallel)_\downarrow \theta(E_F - E_s(\tilde{\mathbf{k}}_\parallel)_\downarrow) \right\} \\ &= \left(\frac{L}{2\pi} \right)^2 \int \frac{\hbar}{2} \left\{ \frac{1}{\hbar} \frac{\partial E_s(\tilde{\mathbf{k}}_\parallel)_\uparrow}{\partial k_y} \theta(E_F - E_s(\tilde{\mathbf{k}}_\parallel)_\uparrow) \right. \\ &\quad \left. - \frac{1}{\hbar} \frac{\partial E_s(\tilde{\mathbf{k}}_\parallel)_\downarrow}{\partial k_y} \theta(E_F - E_s(\tilde{\mathbf{k}}_\parallel)_\downarrow) \right\} d\tilde{k}_x d\tilde{k}_y = 0, \end{aligned}$$

where L is an appropriate length of the period for the evaluation. Thus, in our model the spin current flows spontaneously in the x direction. Being compared with previous study in in-plane inversion asymmetry, this is fundamentally new knowledge which our study brings. This phenomenon can be utilized as a new mechanism to generate the spin current by the use of nonmagnetic materials as

the spin Hall effect, spin-rotation coupling [26], and helical spin polarization of topological insulators [27].

4. Conclusion

We proposed a model of spin-splitting surface states. In our model the spin degeneracy is split from breaking of the twofold symmetry of the surface. We derive these results by $\mathbf{k} \cdot \mathbf{p}$ theory. Additionally, for n-type GaAs the spin current flows in the parallel direction to a mirror plane spontaneously. This phenomenon can be utilized as a new mechanism to generate the spin current.

References

- [1] Sinova J, Culcer D, Niu Q, Sinitsyn NA, Jungwirth T, MacDonald AH. Universal intrinsic spin Hall effect. *Phys Rev Lett* 2004;92:126603.
- [2] Murakami S, Nagaosa N, Zhang S-C. Dissipationless quantum spin current at room temperature. *Science* 2003;301:1348.
- [3] Li Z, Liu X, Xie W, Wu Y. Detectable spin-orbit splitting in Ni doped graphene. *Phys Lett A* 2014;378:3196.
- [4] Dresselhaus G. Spin-orbit coupling effects in zinc blende structures. *Phys Rev* 1955;100:580.
- [5] Bychkov YA, Rashba EI. Properties of a 2D electron gas with lifted spectral degeneracy. *Pis'ma Zh Eksp Theor Fiz* 1984;39:66 [*JETP Lett.* 1984;39:78].
- [6] LaShell S, McDougall BA, Jensen E. Spin splitting of an Au(111) surface state band observed with angle resolved photoelectron spectroscopy. *Phys Rev Lett* 1996;77:3419.
- [7] Vervoort L, Ferreira R, Voisin P. Effects of interface asymmetry on hole subband degeneracies and spin-relaxation rates in quantum wells. *Phys Rev B* 1997;56:R12744.
- [8] Krebs O, Rondi D, Gentner JL, Goldstein L, Voisin P. Inversion asymmetry in heterostructures of zinc-blende semiconductors: interface and external potential versus bulk effects. *Phys Rev Lett* 1998;80:5770.
- [9] Premper J, Trautmann M, Henk J, Bruno P. Spin-orbit splitting in an anisotropic two-dimensional electron gas. *Phys Rev B* 2007;76:073310.
- [10] Ast CR, Henk J, Ernst A, Moreschini L, Falub MC, Pacilé D, Bruno P, Kern K, Grioni M. Giant spin splitting through surface alloying. *Phys Rev Lett* 2007;98:186807.
- [11] Gierz I, Suzuki T, Frantzeskakis E, Pons S, Ostanin S, Ernst A, Henk J, Grioni M, Kern K, Ast CR. Silicon surface with giant spin splitting. *Phys Rev Lett* 2009;103:046803.
- [12] Vajna S, Simon E, Szilva A, Palotas K, Ujfalussy B, Szunyogh L. Higher-order contributions to the Rashba-Bychkov effect with application to the Bi/Ag(111) surface alloy. *Phys Rev B* 2012;85:075404.
- [13] Bernevig BA, Zhang S-C. Quantum spin Hall effect. *Phys Rev Lett* 2006;96:106802.
- [14] Pikus GE, Titkov AN. Optical orientation. North Holland: Amsterdam; 1984 [Chap. 3].
- [15] D'yakonov MI, Marushchak VA, Perel' VI, Titkov AN. The effect of strain on the spin relaxation of conduction electrons in III-V semiconductors. *Zh Eksp Theor Fiz* 1986;90:1123 [*Sov. Phys. JETP* 1986;63:655].
- [16] Bir GL, Pikus GE. Effect of deformation on the energy spectrum and electrical properties of semiconductors of the InSb type. *Fiz Tverd Tela (Leningrad)* 1961;3:3050 [*Sov. Phys. Solid State* 1962;3:2221].
- [17] Howlett W, Zukotynski S. Effect of deformation on the conduction band of III-V semiconductors. *Phys Rev B* 1977;16:3688.
- [18] Bahder TB. Eight-band $\mathbf{k} \cdot \mathbf{p}$ model of strained zinc-blende crystals. *Phys Rev B* 1990;41:11992.
- [19] Wu MW, Jiang JH, Weng MQ. Spin dynamics in semiconductors. *Phys Rep* 2010;493:61.
- [20] Bir GL, Pikus GE. Symmetry and strain-induced effects in semiconductors. New York: John Wiley & Sons; 1974 [Chap. 5].
- [21] Bir GL, Pikus GE. Symmetry and strain-induced effects in semiconductors. New York: John Wiley & Sons; 1974 [Chap. 4].
- [22] Krebs O, Seidel W, André JP, Bertho D, Jouanin C, Voisin P. Investigations of giant ‘forbidden’ optical anisotropy in GaInAs-InP quantum well structures. *Semicond Sci Technol* 1997;12:938.
- [23] Rössler U, Kainz J. Microscopic interface asymmetry and spin-splitting of electron subbands in semiconductor quantum structures. *Solid State Commun* 2002;121:313.
- [24] Krebs O, Voisin P. Giant optical anisotropy of semiconductor heterostructures with no common atom and the quantum-confined pockels effect. *Phys Rev Lett* 1996;77:1829.
- [25] Ivchenko EL, Kaminski AY, Rössler U. Heavy-light hole mixing at zinc-blende (001) interfaces under normal incidence. *Phys Rev B* 1996;54:5852.
- [26] Matsuo M, Ieda J, Harii K, Saitoh E, Maekawa S. Mechanical generation of spin current by spin-rotation coupling. *Phys Rev B* 2013;87:180402(R).
- [27] Brüne C, Roth A, Buhmann H, Hankiewicz EM, Molenkamp LW, Maciejko J, Qi X-L, Zhang S-C. Spin polarization of the quantum spin Hall edge states. *Nat Phys* 2012;8:485.